Simulating the Mechanical Behavior of Metallic Nanowires over Experimentally Accessible Timescales on Roadrunner

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For many years now, we have witnessed explosive growth in our capability to control the structure of materials down to the atomic scale. For example, it is now possible to bring the tip of an atomic force microscope, which might be only a few atoms wide at the apex, in contact with a surface. In the case of a metal tip contacting a metal surface or another tip, a bonded contact forms, and, if the tip is then lifted away from the surface, surface reorganization and diffusion often creates a nanowire that maintains a connection between the tip and surface. This process, as captured by high-resolution transmission electron microscopy, is shown in Fig. 1. This kind of manipulation can be exploited for the intentional creation and study of nanowires, whose width can sometimes be reduced all the way down to a single atomic chain by continuing the retraction process. These nanowires are an ideal probe of the nanoscale behavior of materials, be it mechanical [1] or electrical [2], and hence are of interest both for fundamental studies and because of their expected importance in various nanotechnology applications such as electrical conductors and electrical or mechanical switches. However, a deeper understanding of the fundamental nanoscale behavior of materials is required before these applications can become widespread. Indeed, experiments at the nanoscale are hard to control and sometimes lack the resolution necessary to fully understand how the systems behave. For example, metallic nanowires are often seen to completely disappear from one frame to another, leaving one completely in the dark about the basic mechanisms leading to their failure. Further, the act of imaging itself leads to an uncontrolled increase of the temperature of the wire, making it very difficult to perform these experiments in controlled and reproducible conditions.

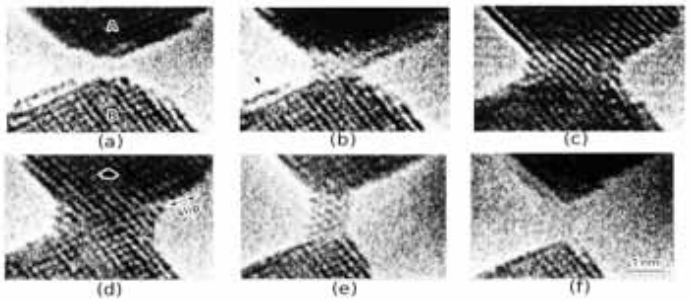

Fig. 1. A series of high resolution transmission electron microscope (HRTEM) images showing the contact formation, retraction, and rupture processes of two gold tips. (a)-(c): contact formation process with (a) corresponding to t=0 s, (b) to t=110/30 s, (c) to t=129/30 s; (d)-(f) retraction and rupture processes: (d)t=0 s, (e)t=2 s, (f) t=3 s. Figures from [1].

There is thus a pressing need for atomistic numerical simulations to complement such experiments and help interpret and understand them. The most powerful tool for performing this kind of simulation is molecular dynamics (MD), whereby one integrates the equations of motion of all the atoms in the system, advancing the positions and velocities of the atoms by repeatedly taking small steps forward in time. In this way, one learns about the evolution of the system with full atomistic detail. However, for many systems and processes we would like to study there is a serious problem with the mismatch in time scale. For example, the nanowire-stretching process discussed above usually takes place over seconds or, at the very fastest, milliseconds. In contrast, conventional MD simulations are limited to a time scale of about one microsecond, even on the fastest parallel computers, i.e., 10^3 to 10^7 times faster than the experimental reality. Because of this extremely large time gap, physical arguments suggest that current simulations do not adequately represent reality.

The way to overcome these limitations is to use so-called Accelerated Molecular Dynamics (AMD) methods to reformulate the problem in a form that is more amenable to computer simulation. For example, the Parallel Replica Dynamics (ParRep) [3] method developed at LANL generates a proper evolution of the system while allowing a parallelization of the problem in the time domain. This allows one to make optimal use of massively parallel computers to reach time scales that are orders of magnitude longer that what could be done with conventional MD. When implemented on petascale supercomputers like Roadrunner, the ParRep method enables one to study the evolution of nanoscale systems (containing about a thousand atoms or so) at the unprecedented rate of about 0.1ms per wall-clock hour when using 12,000 replicas on 120,000 Opteron and IBM Cell Broadband Engine (Cell BE) cores, thereby allowing a direct connection between experiments and fully atomistic simulations.

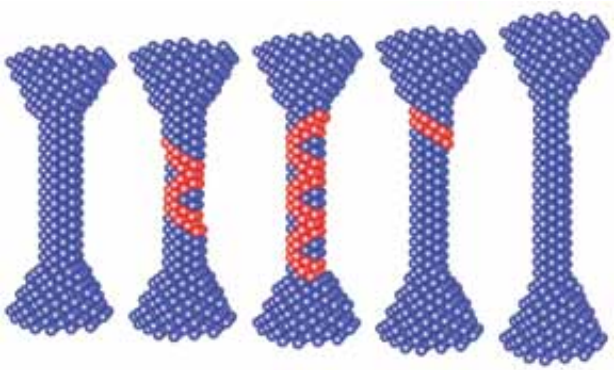

Fig. 2. Early stage of a ParRep simulation of the stretching of a silver nanowire on Roadrunner at a temperature of 300K and a retraction velocity of 10^{-5} m/s. From left to right, t=0 μs, t=30 μs, t=60 μs, t=90 μs, t=150 μs. Atoms in noncrystalline configurations are shown in red.

Using ParRep on Roadrunner, we simulated silver nanowire stretching experiments similar to those illustrated in Fig. 1 for different nanowire sizes, temperatures, and retraction velocity, reaching more than one millisecond of simulation time in a few instances, more than a thousand times longer than conventional techniques would have allowed. Overall, we were able to study the change of behavior of these wires while varying the strain rate by more than four orders of magnitude, a feat that was unthinkable before the advent of Roadrunner.

Thanks to these simulations, a picture of the evolution of these systems is emerging. The basic plastic reaction of the system when subjected to strain is to create stacking faults along (111) planes. These stacking faults are highlighted in red in Fig. 2. The formation of a zig-zag network of such stacking faults causes the release of internal stresses while leading to the elongation and narrowing of the wire. Interestingly, almost all wires, independently of temperature or strain rate, initially behave this way. As the wire is stretched further, given enough time, these stacking faults annihilate, leaving behind a defect-free wire that is uniformly thinned down relative to the initial configuration. These simulations illustrate the unique ability of these nanostructures to, under suitable conditions, heal themselves when subjected to severe external constraints. Note that this self-healing behavior emerges only on long time scales that are completely inaccessible to standard MD simulations.

The later stages of the simulation of the evolution of nanowires also revealed some completely unintuitive mechanisms by which plastic deformation occurs at the nanoscale. As shown in Fig. 3, one of these mechanisms is the conversion of bulk-like segments of the wire into low-symmetry helical structures (here a fivefold-symmetric icosahedral structure). These structures appear to be extremely tolerant to mechanical constraints. Indeed, the conversion process between two relatively stable conformations offers a continuous pathway for the stretching to occur, in contrast with competing mechanisms that lead to the accumulation of defects and ultimately to failure. Through this pathway, elongations in excess of 100% have been observed without failure. Once again this process, involving structures that are not allowed by the symmetry of the bulk crystal, demonstrates the unique ability of nanoscale systems to react to their environment in completely unintuitive ways.

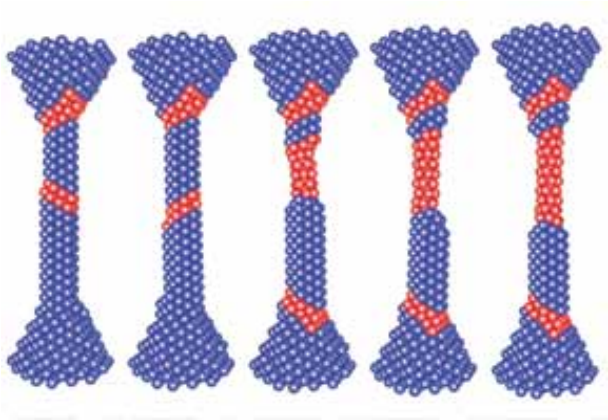

Fig. 3. Late stage of a ParRep simulation of the stretching of a silver nanowire on Roadrunner at a temperature of 300K and a retraction velocity of 10^{-5} m/s. From left to right, t =165 μs, t = 180 μs, t =195 μs, t =210 μs, t =225 μs. Atoms in noncrystalline configurations are shown in red.

The conjunction of innovative algorithms and methods with the unprecedented computational power of Roadrunner enables us to simulate, for the first time, the mechanical behavior of metallic nanowires, which are widely foreseen as playing a major role in the next generation of nano-devices, on experimentally accessible time scales. With this new capability it is now possible to directly assist in the interpretation of experiments as well as in the design of novel structures with precisely tailored properties.

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